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The Features of Bainite Transformation in Alloyed Steels

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Abstract. The main factors affecting the kinetics of isothermal bainite transformation in alloyed steels were determined using the algorithms of the computer modelling of phase transformations in the solid state. The experimental and calculated transformation kinetics was described and compared using well known Kolmogorov-Johnson-Mehl-Avrami (KJMA) equation and Austin-Rickett (AR) equation. The effect of the initial configuration and the nucleation rate of the new phase nuclei on the parameters of the bainite transformation was analysed. The calculated kinetics of phase transformation at different nucleation rates was compared with the experimentally observed for HY-TUF and D6AC steels. The mechanism of the bainite transformation in alloyed steels was explained.

1. Introduction

Discussions about the “mechanism” of the bainite transformation in steels have been going on for a long time, since the discovery of the bainite by Davenport and Bain in the 1930s [1]. However, despite the critical differences, some of the distinguishing features of the bainite transformation in steels are not in doubt. These features consist in the differentiation of the bainite morphology into “upper” and “lower”, in the presence of the temperature of the onset of the bainite transformation, B_s , and in the incompleteness of the bainite transformation [2–4].

Currently, there are two main concepts that explain the nature of bainite transformation. The first one considers the nucleation and growth of bainite as a diffusion-controlled process of increment growth of the “ledges” at the interface between α -plates and the surrounding austenite. The second concept is based on a diffusionless transformation, when the bainite is formed by successive autocatalytic nucleation and growth of α -subunits.

The morphological classification of bainite into “upper” and “lower” made it possible to combine two different concepts of the bainite formation: it is believed that the upper bainite is formed mainly due to the diffusion, and the lower bainite is formed by the shear rearrangement of the crystal lattice [5]. However, in the literature there are other varieties of bainite [6–8], for example, granular, columnar, etc., formation of which is not yet explained.

2. Experimental

The commercial alloyed steels HY-TUF and D6AC were studied (the chemical composition is listed in Table 1).

The experimental kinetics of isothermal bainite transformation in the HY-TUF and D6AC steels was studied using LINSEIS L78 “R.I.T.A.” dilatometer. The heating temperature of the steel specimens (diameter 4 mm, length 10 mm) was 925 °C, the holding time was 15 minutes. The cooling rate to the isothermal transformation temperature was 30 °C/s in order to prevent the austenite



transformation before the required temperature was reached. The isothermal holding time at a temperature in the range of 300...500 °C was 2...4 hours. As a result, the dependences of the bainite fraction on the time were obtained.

Table 1. The chemical composition of the studied steels, wt. %

Steel	C	Cr	Mn	Si	Ni	Mo	V
HY-TUF [9]	0.24	0.31	1.35	1.42	1.71	0.40	0.01
D6AC [10]	0.49	1.11	0.79	0.23	0.46	0.98	0.11

The mathematical description of the experimental kinetics of the isothermal austenite transformation was carried out using Kolmogorov-Johnson-Mehl-Avrami (KJMA) equation (1) [11–15] and Austin-Rickett (AR) equation (2) [16]:

$$P = 1 - e^{-k\tau^n}, \quad (1)$$

$$P = 1 - \frac{1}{1 + k\tau^n}, \quad (2)$$

where P – the austenite transformation fraction; τ – time, s; k – temperature-dependent parameter; n – exponent.

Computer simulation of the phase transformation was implemented using the MATLAB® software. The software package was developed on the basis of the procedures for constructing the wave fronts in an isotropic medium [17]. The simulation method is described in detail in [18].

The results of the analysis of the experimental and simulated transformation kinetics were presented as the kinetic curves in the logarithmic coordinates “ $\ln(-\ln(1-P))-\ln(\tau)$ ” and “ $\ln[P/(1-P)]-\ln(\tau)$ ” in the case of the equations KJMA (1) and AR (2), respectively.

3. Results and discussion

The experimental kinetics of the isothermal bainite transformation in the studied steels at different temperatures (lower and upper bainite range) are shown in Figure 1 and 2. Figure 2 depicts the transformation kinetics in the logarithmic coordinates of the KJMA (1) and AR (2) equations. Note that in the majority of cases, the KJMA kinetics showed an inflection, characterized by a change in the value of exponent n . The only exception is the formation of upper bainite in D6AC steel (Figure 2, c) where the KJMA kinetics had a linear form. In turn, the AR kinetics had a linear form in the majority of cases except the one for the upper bainite in D6AC steel at 420 °C (Figure 2, d): in this case, an explicit inflection was observed on the AR kinetic curve.

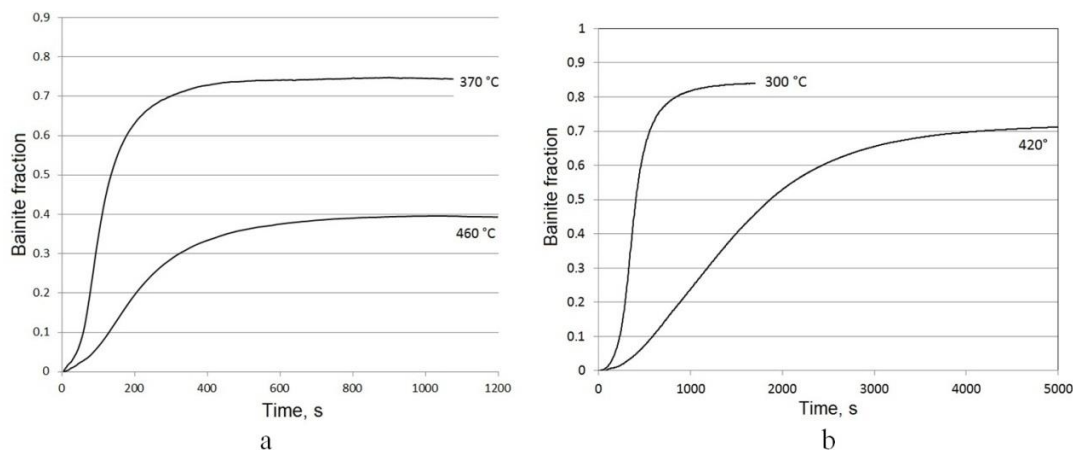


Figure 1. Experimental kinetics of isothermal bainite transformation in steels HY-TUF (a) and D6AC (b).

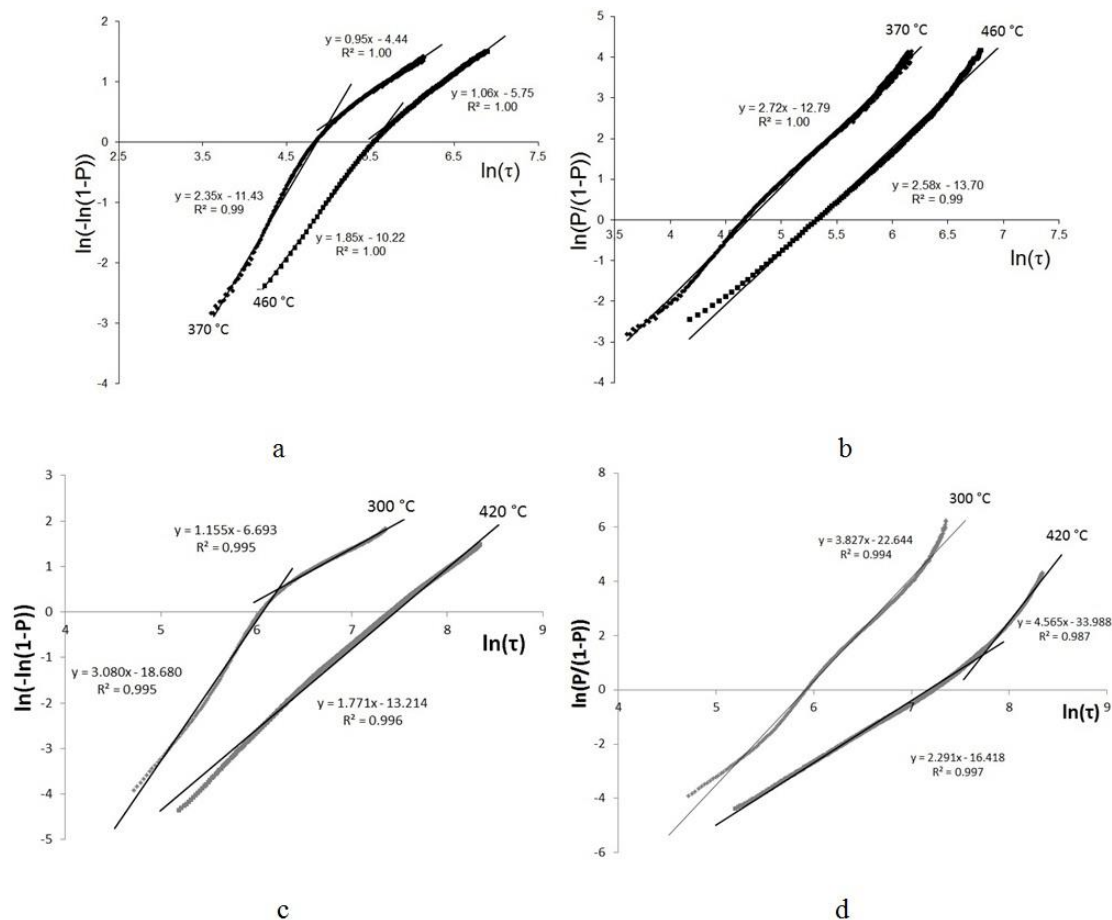


Figure 2. Kinetic curves of isothermal bainite transformation in logarithmic coordinates for steels HY-TUF (a, b), D6AC (c, d): a, c) KJMA equation; b, d) AR equation.

The degree of linearity of the kinetic curve reflects the adequacy of the mathematical description of the entire process of isothermal transformation if the constant coefficients of Equations (1) and (2) are used. To characterize the adequacy of the mathematical description of the observed kinetics of transformation, we used the sum of the squared differences between the experimental and calculated fractions of bainite at each moment of time in the range of the bainite fraction 0.02...0.98. It was found that the AR equation provides up to 40 times better description of the experimental kinetics of bainite transformation compared to the KJMA equation, except for the transformation in D6AC steel at 420 °C. Thus, there are some conditions of the bainite transformation that determine the nature of the process, and these conditions can depend both on the temperature of the transformation and on the chemical composition of the steel. For example, D6AC steel contains more carbide-forming elements (Mo, V) than HY-TUF steel, and the latter contains a significant amount of silicon and nickel (up to 2 wt.%).

To understand the physical phenomena behind the change in the nature of the bainite transformation, a computer simulation of the phase transformation was carried out.

First of all, the calculation was performed for the number of the new phase nuclei randomly distributed in the virtual volume: the average concentration of the new phase nuclei at the beginning of the calculation was 1.25×10^{-2} %, the nucleation rate of the new phase was assumed to be 0. The simulation results showed that the description of the kinetics of the phase transition by the KJMA equation gave a satisfactory result throughout the entire transformation (Figure 3, a). The kinetic curve had a linear form, the exponent of the KJMA equation is $n \approx 3$, and the value $\ln(k) \approx -13.56$. The

obtained value of the exponent n is consistent with the classical theory of phase transformations [19, 20], which relates the exponent n of the KJMA equation to the shape of the growing particles of a new phase (in this work, three-dimensional growth of nuclei leads to the growth of quasispherical particles).

When a concentration gradient of nuclei in the virtual volume was applied, a substantially different kinetics of the phase transition was observed (Figure 3, b). From the beginning of the transformation to the fraction 0.60...0.65, the exponent n was 2.8, and $\ln(k)$ was -11.0 . These values are close to the ones obtained previously for the random distributed nuclei. Upon reaching the transformed fraction 0.60...0.65, an inflection of the kinetic curve was observed, and the transformation proceeded with another parameters: $n = 1.3$; $\ln(k) = -5.2$. The obtained values of the parameters of the KJMA equation satisfactorily coincide with the values obtained for the experimentally observed kinetics of bainite transformation in the steels under study. Note, that the kinetic curves in the AR coordinates have exactly the opposite characteristics: for the uniform nuclei distribution an inflection is observed on the kinetic curve (Figure 4, a), for the concentration gradient of the nuclei the kinetic curve has a linear form (Figure 4, b). Thus, the nature of the bainite transformation in steel of a certain composition depends on the distribution pattern of the critical nuclei able to grow at a specific temperature.

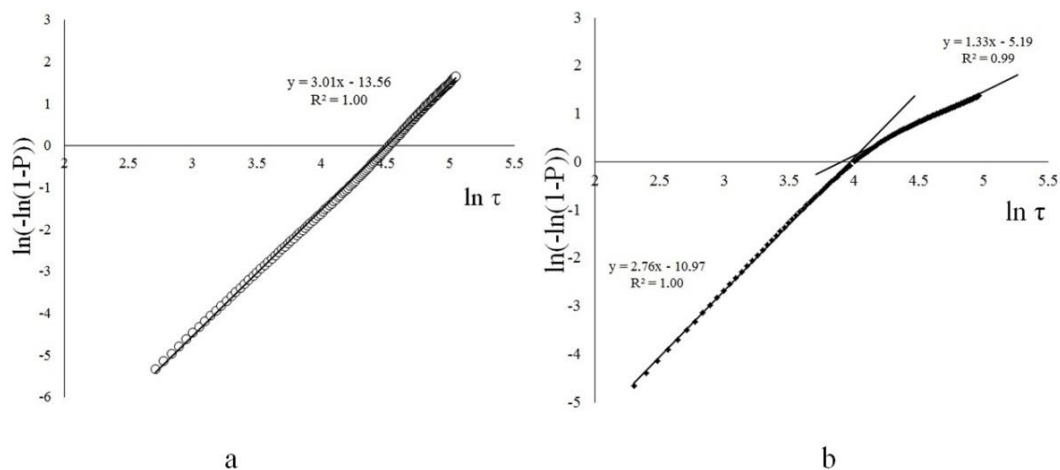


Figure 3. Kinetic curve of the simulated phase transition obtained for the different initial distribution of the new phase nuclei (KJMA equation, zero nucleation rate): a) random; b) concentration gradient.

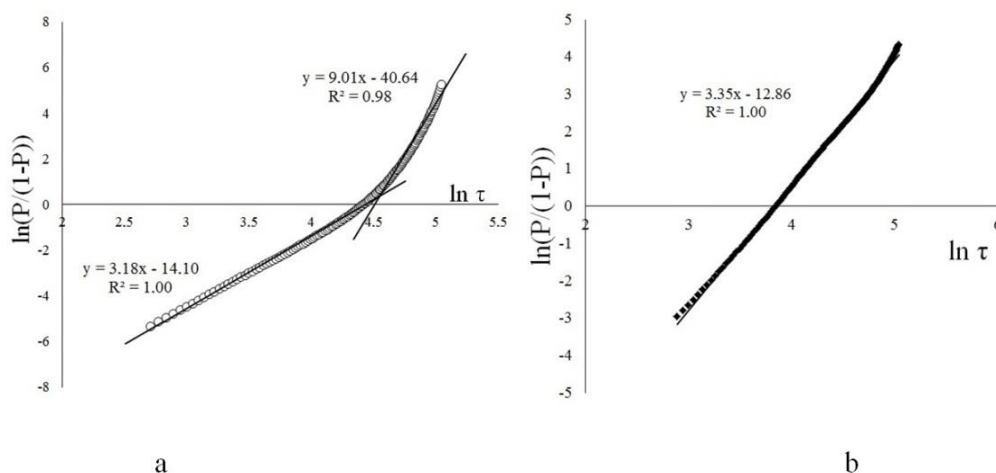


Figure 4. Kinetic curve of the simulated phase transition obtained for the different initial distribution of the new phase nuclei (AR equation, zero nucleation rate): a) random; b) concentration gradient.

The effect of the nucleation rate on the transformation process was evaluated. From 1 to 10 new nuclei of the second phase were added into the virtual volume at every calculation step. It was found that the increase in the nucleation rate led to the linearization of the KJMA kinetics (Figure 5, a), and a characteristic inflection appeared on the AR kinetics (Figure 5, b). So, the adequacy of the description of the transformation kinetics by the AR equation decreased.

Since the AR equation is most suitable for the description of the experimental kinetics of isothermal bainite transformation in the majority of cases, it is most likely that during the bainite transformation in the studied steels there were no nucleation of new nuclei. In this case, the transformation proceeded only due to the growth of the nuclei formed in the volume of the austenite during cooling from the austenization temperature to the temperature of isothermal holding below B_s . Thus, at the initial stage the bainite transformation is similar to the martensite transformation: supercooling below the B_s temperature leads to the formation of a certain number of nuclei depending on the degree of supercooling. Subsequently, these nuclei grow by layers, uniformly, which is characteristic of a diffusion-controlled process, and new nuclei do not form during the transformation.

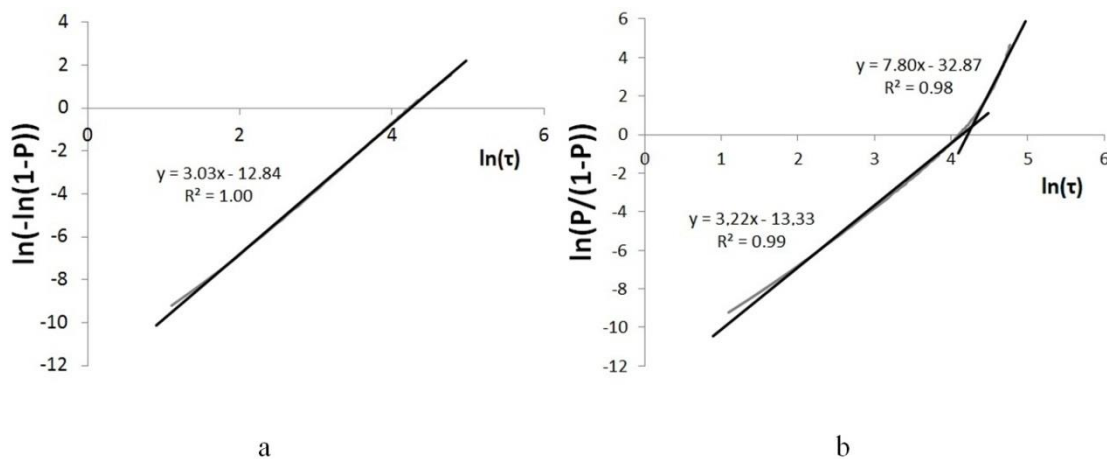


Figure 5. Kinetic curves of the simulated phase transition (concentration gradient of the nuclei, nucleation rate 5 nuclei per cycle): a) KJMA equation; b) AR equation.

In the case of the upper bainite formation in D6AC steel (Figure 2, c, d), the nature of the transformation is similar to the diffusion-controlled growth at a nonzero nucleation rate. This is due to the carbide formation during the isothermal treatment, since D6AC steel contains a large amount of the carbide-forming elements and does not contain a sufficient amount of silicon, which suppresses the precipitation of carbides. Dispersed carbides precipitated from the austenite can serve as the substrates or additional nuclei for the growth of the bainite colonies.

4. Conclusions

The kinetics of isothermal bainite transformation in steels HY-TUF and D6AC at the temperature of lower and upper bainite formation was studied. It was found that the lower and upper bainite transformation in HY-TUF steel is adequately described by the Austin-Rickett equation. For D6AC steel the Austin-Rickett equation was suitable only for the formation of lower bainite. The kinetics of the upper bainite formation in D6AC steel was adequately described by the KJMA equation.

The computer simulation showed that the initial distribution of new phase nuclei in the virtual volume and the nucleation rate had a significant effect on the kinetics of the phase transformation.

It was shown that the bainite transformation in steel occurred under the following conditions: initial uneven distribution of nuclei, layer-by-layer growth, lack of formation of new nuclei during the transformation. Thus, the bainite transformation combines the features of a martensite transformation (the formation of a certain number of nuclei depending on the degree of supercooling below the

equilibrium temperature B_s) and diffusion-controlled transformation (uniform layer-by-layer growth of nuclei).

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Acknowledgments

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